

# Anderson localization of polaron states

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Using the vanishing of the typical polaron tunneling rate as an indicator of the breakdown of itinerancy, we study the localization of polaron states in a generic model for a disordered polaronic material. We find that extremely small disorder causes an Anderson localization of small polaron states. However, the ratio between the critical disorder strength needed to localize all states in the polaron band and the renormalized bandwidth is not necessarily smaller than for a bare electron.

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The polaron concept has played a central role in the analysis of strongly coupled electron-phonon (EP) systems since the pioneering work of Landau. [1] Nevertheless, even fundamental properties of a polaron are not yet completely understood, especially with respect to the effect of disorder. Polaron signatures are currently discussed in compounds such as the colossal magnetoresistance manganites [2], the charge ordered nickelates and bismuthates [3], and molecular organic semiconductors [4] –all *complex* materials, where imperfections potentially play an important role.

The essence of polaron formation is the crossover from a weakly (phonon) dressed charge carrier to a strongly mass-enhanced, less mobile polaronic quasiparticle with increasing EP coupling strength. [5, 6] This process is usually called *self-trapping*, since the distortion that tends to bind the carrier in a deformable lattice is induced by the carrier itself, i.e., the trapping potential depends on the state of the carrier. [7] Nonetheless, even if the carrier is “confined” to a single lattice site (small polaron), this type of trapping *does not imply localization*. The tunneling between different lattice sites is still relevant and a self-trapped carrier resides in an itinerant polaron state. [6] On the other hand, it is well known that for sufficiently strong randomness the itinerancy of (single electron) states is destroyed and the states are Anderson localized. [8, 9] Obviously, disorder will affect the itinerancy of polaron states. Likewise, it was suggested that the “mobility edge”, separating itinerant (extended) and localized states, will be strongly influenced by the EP interaction [10]. At the moment, however, despite its apparent relevance for various transport processes in polaronic materials, little is known rigorously about how Anderson localization affects polaron states, and vice versa.

As a first step toward addressing this problem, in Ref. [11] a single polaron in a Holstein model with site-diagonal, binary-alloy-type disorder was studied within the dynamical mean field approximation (DMFA). [12] The DMFA, however, cannot (fully) discriminate between itinerant and localized states (as shown below), mainly because the randomness is treated at the level of the coherent potential approximation. [13]

The purpose of this paper is to remedy this shortcoming, and to present an advanced theory that is capable of describing both the Anderson localization and self-trapping phenomena. As a generic model we consider the single-particle Anderson-Holstein Hamiltonian

$$\mathcal{H} = \sum_i \epsilon_i n_i - J \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.}) - \sqrt{E_p \Omega} \sum_i (b_i + b_i^\dagger) n_i + \Omega \sum_i b_i^\dagger b_i, \quad (1)$$

where  $J$  is the electron transfer amplitude between neighboring sites,  $\Omega$  denotes the bare frequency of the optical phonon ( $\hbar = 1$ ), and  $E_p$  is the polaron shift. In Eq. (1), the on-site energies  $\{\epsilon_i\}$  are assumed to be independent, identically distributed random variables with a probability density  $p(\epsilon_i) = (1/\gamma)\theta(\gamma/2 - |\epsilon_i|)$ .

Without disorder, the physical properties of the Holstein model are governed by three parameter ratios: the adiabaticity  $\alpha = \Omega/J$  [determining whether the electron is light ( $\alpha \ll 1$ ) or heavy ( $\alpha \gg 1$ ) (Ref. [7])], and two dimensionless EP coupling constants  $\lambda = E_p/2J$  and  $g^2 = E_p/\Omega$ . Extensive numerical studies of the Holstein model on finite one-dimensional (1D) and 2D lattices have shown that polaron formation sets in if two conditions  $\lambda \gtrsim 1$  and  $g^2 \gtrsim 1$  are fulfilled. [14, 15, 16] The internal structure of the polaron depends on  $\lambda$  and  $\alpha$ . As a result, disorder affects polaron states quite differently in the adiabatic ( $\alpha \ll 1$ ), nonadiabatic ( $\alpha \sim 1$ ), and antiadiabatic ( $\alpha \gg 1$ ) cases. Furthermore, in the crossover region, where polaron formation sets in, long-range tunneling induced by the EP coupling [15] is expected to decrease the tendency toward localization.

To analyze the effects of disorder on polaron formation quantitatively, we adopt the recently developed statistical DMFA (statDMFA) (Ref. [17]) to the Anderson-Holstein model. This method is an extension of the self-consistent theory of localization of bare electrons [18] to models with interactions, which has been successfully applied, e.g., to the disordered Hubbard [17] and Anderson lattice [19] models. The statDMFA is essentially a probabilistic method, based on the self-consistent construction of random samples for the (local) physical quantities of

interest.

The statDMFA is conveniently constructed for a Bethe lattice with finite connectivity  $K$ . For later purposes, we rescale the transfer amplitude  $J \rightarrow \tilde{J}/\sqrt{K}$  and define  $\tilde{\lambda} = E_p/2\tilde{J}$  and  $\tilde{\alpha} = \Omega/\tilde{J}$ . Applying the statDMFA (Ref. [17]) to model (1), the local zero-temperature single-electron Green function reads  $\mathcal{G}_i(z) = [z - \epsilon_i - H_i(z) - \Sigma_i(z)]^{-1}$  ( $z = \omega + i\eta$ ), with the EP self-energy  $\Sigma_i(z)$  and the hybridization function

$$H_i(z) = \frac{\tilde{J}^2}{K} \sum_{j=1}^K \frac{1}{z - \epsilon_j - H_j(z) - \Sigma_j(z)}. \quad (2)$$

In the spirit of the self-consistent theory of localization, [18] the statDMFA ignores that the functions on the right-hand side of Eq. (2) should be calculated for the Bethe lattice with the site  $i$  removed. It furthermore takes  $K$  as the typical number of terms, although for the initial site there would be  $K+1$  terms. As a consequence, the bare local density of states (LDOS) becomes semi-elliptic (with a half-band-width  $\tilde{W}_0/2 = 2\tilde{J}$ ), irrespective of the value of  $K$ , which makes the mean field character of the statDMFA evident. [20]

The most severe approximation within the statDMFA is related to the calculation of  $\Sigma_i(z)$ . Although the connectivity of the Bethe lattice is finite in Eq. (2), the self-energy is determined as if the Bethe lattice had infinite connectivity. [21] The self-energy is then local (as in the DMFA), [11, 22] and reads  $\Sigma_i(z) = E_p 1\Omega / ([F_i^{(1)}(z)]^{-1} - E_p 2\Omega / \dots)$  with  $[F_i^{(p)}(z)]^{-1} = z - p\Omega - \epsilon_i - H_i^{(p)}(z)$  and  $H_i^{(p)}(z) = H_i(z - p\Omega)$ . Here the energy shift keeps track of the number of virtual phonons, and the index  $p$  is a positive integer, because of the absence of thermally excited phonons.

A natural measure of the itinerancy of a polaron state is the tunneling rate from a given site defined as the imaginary part of the hybridization function  $\Gamma_i(\omega) = (\pi\tilde{J}^2/K) \sum_{j=1}^K N_j(\omega)$ , where  $N_j(\omega) = -(1/\pi)\text{Im}\mathcal{G}_j(\omega)$  is the LDOS. A vanishing tunneling rate  $\Gamma_i(\omega)$  implies a localized state at energy  $\omega$ .

Due to the randomness in the on-site energies, the tunneling rate  $\Gamma_i(\omega)$  is a random variable, and the question of whether it vanishes or not depends on the probability density exhibiting, quite generally, characteristic differences for itinerant and localized states. [8, 18] For an itinerant state, the probability density is narrow and (approximately) symmetric. Thus, the most probable value and the arithmetic mean (average),  $\Gamma^{\text{av}}(\omega) = (1/N) \sum_i \Gamma_i(\omega)$ ,  $N$  being the total number of lattice sites, are almost identical and  $\Gamma^{\text{av}}(\omega)$  will be a good estimate for the tunneling rate. On the other hand, for a localized state, the probability density is very wide with an extremely long tail toward large values, implying that the most probable value is much smaller than the aver-

age. In that case, the geometric mean (typical value)

$$\Gamma^{\text{typ}}(\omega) = \exp \left[ \frac{1}{N} \sum_i \log \Gamma_i(\omega) \right] \quad (3)$$

seems to be a more appropriate estimate of the tunneling rate. Accordingly, a vanishing *typical* (rather than average) tunneling rate should be taken as a localization criterion. [18]

The typical tunneling rate is most directly calculated from a recursion scheme for the hybridization function

$$H_i^{(p)} = \frac{\tilde{J}^2}{K} \sum_{l=1}^K \frac{1}{[F_l^{(p)}]^{-1} - \frac{E_p 1\Omega}{[F_l^{(p+1)}]^{-1} - \frac{E_p 2\Omega}{\dots}}}. \quad (4)$$

Demanding that  $H_i^{(p)}(z)$  are independent, identically distributed random variables, Eq. (4) can be used to construct a random sample  $\{H_i^{(p)}(z)\}$  ( $i = 1, \dots, N$  and  $p = 0, 1, \dots, M$ ) for the hybridization function, starting from an initial random configuration which is successively updated with a sampling technique similar to the one described in Ref. [18]. More precisely, we are constructing a self-consistent random sample because the probability density for  $H_i^{(p)}(z)$  is assumed to be the same on both sides of Eq. (4). Clearly, the larger  $N$  the better the statistics. A correct description of the polaron effect requires the cutoff  $M$  for the continued fraction to be much larger than the average number of phonons bound in the polaron. Specifically, for the results presented in this paper  $N = 50\,000$  and  $M = 35$ .

It is instructive to consider Eq. (4) for  $K = \infty$ . Applying the law of large numbers shows that  $H_i^{(p)}(z)$  can be replaced by its average  $H^{\text{av}(p)}(z)$ . Then,  $(1/K) \sum_l^K (\dots)$  denotes the (sample) average solely over  $\epsilon_l$ , and Eq. (4) reduces to the DMFA equation for  $H^{\text{av}(p)}(z)$ . (The scaling of  $J$  makes this point particularly clear.) Obviously, the tunneling rate is then  $\pi\tilde{J}^2 N^{\text{av}}(z)$ , i.e., it is proportional to the average LDOS, which is always finite, irrespective of whether the state at energy  $\omega$  is itinerant or localized. [8, 9] Thus, for  $K = \infty$ , i.e., in the DMFA, itinerant and localized states cannot be distinguished.

In the following we present representative numerical results for  $K = 2$  and  $\eta = 10^{-8}$ . We start our discussion with the (nonadiabatic-to-antiadiabatic) weak EP coupling regime. Figure 1 displays typical tunneling rates  $\Gamma^{\text{typ}}(\omega; \gamma)$  as a function of disorder strength  $\gamma$  for two energies  $\omega$ , one below and one above the optical-phonon emission threshold, which, due to the large value of  $\tilde{\alpha}$ , lies far inside the band (see the inset). Below the threshold,  $\text{Im}\Sigma(\omega) = 0$  and the states are coherent. Above the threshold, however, inelastic polaron-phonon scattering yields  $\text{Im}\Sigma(\omega) \neq 0$ , i.e., the states are incoherent, implying that the quantum interference needed for localization [23] is significantly suppressed. We therefore expect the critical disorder strength  $\gamma_c$ , for which  $\Gamma^{\text{typ}}(\omega; \gamma)$  vanishes, to be larger above the phonon emission threshold

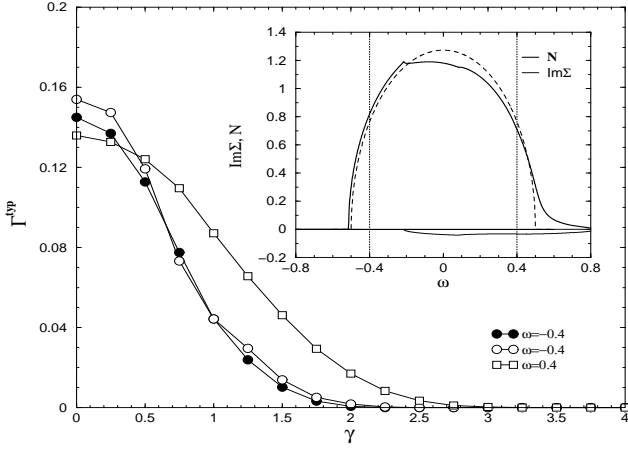


FIG. 1: Typical tunneling rates  $\Gamma^{\text{typ}}(\omega; \gamma)$  in the (non-to-antiadiabatic) weak EP coupling regime ( $\tilde{W}_0 = 1.0$ ,  $\tilde{\alpha} = 1.2$ , and  $\tilde{\lambda} = 0.067$ ). Filled circles denote data for  $\tilde{\lambda} = 0$ . The inset shows the LDOS  $N(\omega)$  and the imaginary part of the EP self-energy  $\text{Im}\Sigma(\omega)$  for  $\gamma = 0$ ; dashed and (vertical) dotted lines indicate, respectively, the density of states for  $\tilde{\lambda} = 0$  and the energies  $\omega$  for which  $\Gamma^{\text{typ}}(\omega; \gamma)$  is plotted.

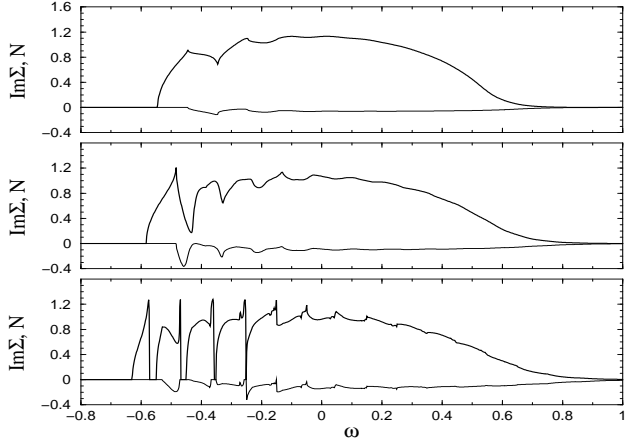


FIG. 2: Evolution of the LDOS  $N(\omega)$  (thick line) and the imaginary part of the EP self-energy  $\text{Im}\Sigma(\omega)$  (thin line) for the ordered Holstein model ( $\gamma = 0$ ) with increasing EP coupling  $\tilde{\lambda} = 0.4, 0.7$ , and  $1.0$  (from top to bottom). Results are given for  $\tilde{\alpha} = 0.4$  and  $\tilde{W}_0 = 1.0$ .

than below it. Indeed, we find  $(\gamma_c/\tilde{W}_0)_{\omega=-0.4} \approx 2.25$  and  $(\gamma_c/\tilde{W}_0)_{\omega=0.4} \approx 3.0$ . It is rather encouraging that the statDMFA recovers this basic feature of the physics of localization. Since the EP coupling is weak the states below the threshold are basically bare electron states and  $(\gamma_c/\tilde{W}_0)_{\omega=-0.4} \approx (\gamma_c/\tilde{W}_0)_{\omega=0.4}^{\tilde{\lambda}=0} \approx 2.0$ , the corresponding ratio for a bare electron. [24]

Increasing the EP coupling, polaron formation starts and the LDOS fragments into an increasing number of (more or less) coherent subbands. [22] Figure 2 illustrates, for the ordered Holstein model ( $\gamma = 0$ ), the evo-

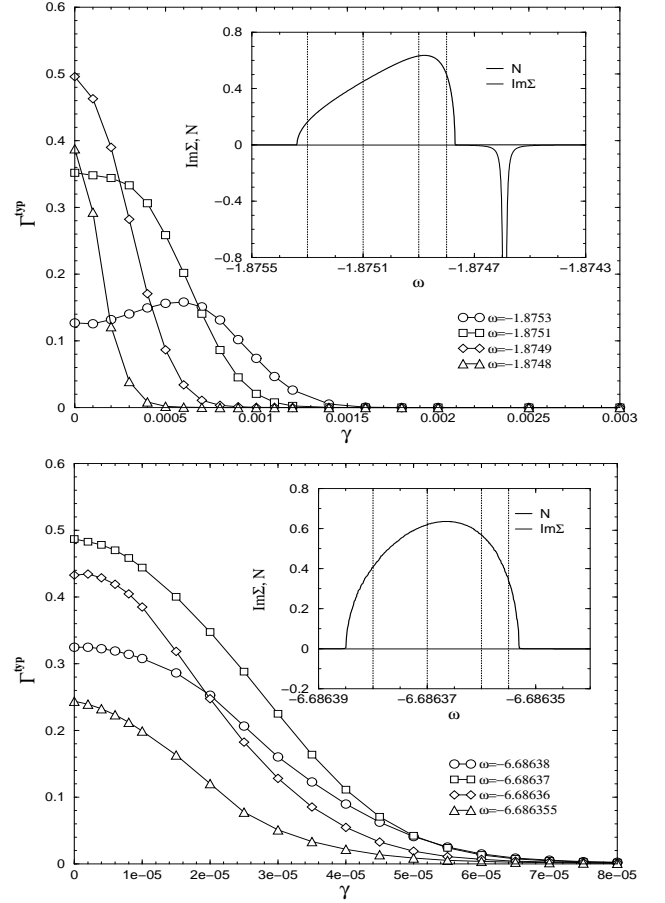


FIG. 3: The upper and lower panels show, respectively, typical tunneling rates  $\Gamma^{\text{typ}}(\omega; \gamma)$  in the (adiabatic) intermediate ( $\tilde{\alpha} = 0.4$ ,  $\tilde{\lambda} = 1.8$ ) and (non-to-antiadiabatic) strong EP coupling regime ( $\tilde{\alpha} = 1.2$  and  $\tilde{\lambda} = 6.6\bar{6}$ ) using  $\tilde{W}_0 = 2.0$ . The insets display the subband LDOS  $N(\omega)$  and the imaginary part of the EP self-energy  $\text{Im}\Sigma(\omega)$  for  $\gamma = 0$  (vertical dotted lines indicate the energies  $\omega$  for which  $\Gamma^{\text{typ}}(\omega; \gamma)$  is plotted). Note the small spectral weight of the lowest polaron subband.

lution of the LDOS with increasing EP coupling  $\tilde{\lambda}$  for fixed  $\tilde{\alpha}$  and  $\tilde{W}_0$ . As far as localization is concerned, the lowest subband is of particular interest, because it is completely coherent and the quantum interference needed for localization is not masked by inelastic polaron-phonon scattering. Numerical studies of the ordered Holstein model demonstrated that the band dispersion of the lowest subband depends on both  $\tilde{\lambda}$  and  $\tilde{\alpha}$ , and may differ significantly from the rescaled bare band. [14, 15] Specifically, the states at the bottom of the subband are mostly electronic and rather mobile due to long-range tunneling induced by EP coupling, whereas the states at the top of the subband are rather phononic and immobile. [15] Therefore, we expect that the critical disorder strength needed to localize states at the top of the subband is much smaller than for states at the bottom. This behavior should be most pronounced in the (adiabatic) intermediate EP coupling regime.

The upper panel of Fig. 3, showing typical tunneling rates  $\Gamma^{\text{typ}}(\omega; \gamma)$  as a function of disorder strength  $\gamma$  for the lowest polaron subband, impressively confirms this striking behavior. The strong asymmetry of the LDOS (see the inset) is a direct consequence of the “hybridization” with the (optical) phonon branch, leading to a band flattening at the Brillouin-zone boundary. As can be seen, states at the zone boundary are very susceptible to disorder and the critical disorder strength  $\gamma_c$  for which  $\Gamma^{\text{typ}}(\omega; \gamma)$  vanishes is substantially smaller than at the bottom of the subband. Clearly, the absolute scale of disorder affecting the subband is on the order of the subband width  $\tilde{W}_1$ , which is strongly renormalized in comparison with the bare band width  $\tilde{W}_0$ . Different from the pure Anderson model, the critical disorder strength needed to localize *all* states of the subband is determined by the states at the bottom (not at the center). We find  $(\gamma_c/\tilde{W}_1)_{\text{complete}} \approx 2.8$ , which is larger than the corresponding ratio for a bare electron  $[(\gamma_c/\tilde{W}_0)_{\text{complete}} \approx 2.25]$  because of the long-range tunneling induced by the EP coupling. Thus, contrary to naive expectations, in the intermediate-coupling (crossover) regime, a polaron is more difficult to localize than a bare electron.

Finally, in the lower panel of Fig. 3, we present typical tunneling rates  $\Gamma^{\text{typ}}(\omega; \gamma)$  in the (nonadiabatic-to-antiadiabatic) strong EP coupling regime. The phonon admixture of the polaron states within the lowest subband is now nearly energy independent. Concomitantly, long-range tunneling as well as band flattening are negligible and the LDOS is rather symmetric (see the in-

set). [15] Accordingly, disorder should affect all the states within the subband more or less equally. Indeed, the critical disorder strength  $\gamma_c$  for which  $\Gamma^{\text{typ}}(\omega; \gamma)$  vanishes is now almost energy independent. We find  $(\gamma_c/\tilde{W}_1)_{\text{complete}} \approx 2.5$ , which is smaller than the ratio for intermediate EP coupling, indicating that in the extreme strong EP coupling adiabatic ( $\tilde{\lambda} \gg 1$ ) and nonadiabatic-to-antiadiabatic ( $g^2 \gg 1$ ) regimes  $(\gamma_c/\tilde{W}_1)_{\text{complete}}$  approaches the corresponding ratio for a bare electron. Here, the band collapse does only change the overall energy scales.

To summarize, we presented, as a first step toward a transport theory for disordered polaronic materials, a theoretical approach capable of describing polaron formation and Anderson localization. We showed that the typical tunneling rate from a given site is an appropriate quantity in order to distinguish itinerant and localized polaron states. Focusing on the disorder-induced localization of a single polaron in the intermediate-to-strong EP coupling regime, we found that extremely small material imperfections turn itinerant polaron states into localized polaron states, suggesting that in real materials (small) polarons are presumably always localized. In the crossover regime, the critical disorder strength, in units of the subband width, needed to localize all states of the lowest polaron subband can be larger than that for the pure Anderson model. From this perspective, disorder-induced localization of a polaron is not necessarily easier than localization of a bare electron.

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